



chain nodes :

24 25 26 27 28 29 30 31 32 33 34 35 36 37

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23

chain bonds :

1-35 11-23 13-37 15-27 15-31 20-24 24-25 24-26 27-28 27-36 28-29 29-30 31-32 32-33 32-34

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13 13-14 13-15 14-17
15-16 16-17 18-19 18-23 19-20 20-21 21-22 22-23

exact/norm bonds :

1-35 15-31 20-24 24-25 24-26 27-36 28-29 29-30 31-32 32-34

exact bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-11 8-9 8-14 9-10 11-12 11-23 12-13 13-14 13-15
13-37 14-17 15-16 15-27 16-17 27-28 32-33

normalized bonds :

18-19 18-23 19-20 20-21 21-22 22-23

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
24:CLASS25:CLASS26:CLASS27:CLASS28:CLASS29:CLASS30:CLASS31:CLASS32:CLASS33:CLASS
34:CLASS